Package ‘sundialr’

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Type Package

Title An Interface to 'SUNDIALS' Ordinary Differential Equation (ODE) Solvers

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Maintainer Satyaprakash Nayak <sn248@cornell.edu>

URL https://github.com/sn248/sundialr

BugReports https://github.com/sn248/sundialr/issues

Description Provides a way to call the functions in 'SUNDIALS' C ODE solving library (<https://computation.llnl.gov/projects/sundials>). Currently the serial version of ODE solver, 'CVODE', sensitivity calculator 'CVODES' and differential algebraic solver 'IDA' from the 'SUNDIALS' library are implemented. The package requires ODE to be written as an 'R' or 'Rcpp' function and does not require the 'SUNDIALS' library to be installed on the local machine.

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LazyData TRUE

Imports Rcpp (>= 0.12.5)

LinkingTo Rcpp, RcppArmadillo

RoxygenNote 7.1.0

Suggests knitr, rmarkdown, testthat

VignetteBuilder knitr

NeedsCompilation yes

Author Satyaprakash Nayak [aut, cre, cph]
(<https://orcid.org/0000-0001-7225-1317>),
Lawrence Livermore National Security [cph],
Southern Methodist University [cph]

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cvode *cvode*

Description

CVODE solver to solve stiff ODEs

Usage

```
cvode(
  time_vector,
  IC,
  input_function,
  Parameters,
  reltolerance = 1e-04,
  abstolerance = 1e-04
)
```

Arguments

`time_vector`	time vector
`IC`	Initial Conditions
`input_function`	Right Hand Side function of ODEs
`Parameters`	Parameters input to ODEs
`reltolerance`	Relative Tolerance (a scalar, default value = 1e-04)
`abstolerance`	Absolute Tolerance (a scalar or vector with length equal to ydot, default = 1e-04)

Examples

```
# Example of solving a set of ODEs with cvode function
# ODEs described by an R function
ODE_R <- function(t, y, p){

  # vector containing the right hand side gradients
  ydot = vector(mode = "numeric", length = length(y))

  # R indices start from 1
  ydot[1] = -p[1]*y[1] + p[2]*y[2]*y[3]
  ydot[2] = p[1]*y[1] - p[2]*y[2]*y[3] - p[3]*y[2]*y[2]
  ydot[3] = p[3]*y[2]*y[2]

  # ydot[1] = -0.04 * y[1] + 10000 * y[2] * y[3]
  # ydot[3] = 30000000 * y[2] * y[2]
  # ydot[2] = -ydot[1] - ydot[3]

  ydot

}

# ODEs can also be described using Rcpp
Rcpp::sourceCpp(code = '

                #include <Rcpp.h>
                using namespace Rcpp;

                // ODE functions defined using Rcpp
                // [[Rcpp::export]]
                NumericVector ODE_Rcpp (double t, NumericVector y, NumericVector p){

                // Initialize ydot filled with zeros
                NumericVector ydot(y.length());

                ydot[0] = -p[0]*y[0] + p[1]*y[1]*y[2];
                ydot[1] = p[0]*y[0] - p[1]*y[1]*y[2] - p[2]*y[1]*y[1];
                ydot[2] = p[2]*y[1]*y[1];

                return ydot;

                }')



# R code to genrate time vector, IC and solve the equations
time_vec <- c(0.0, 0.4, 4.0, 40.0, 4E2, 4E3, 4E4, 4E5, 4E6, 4E7, 4E8, 4E9, 4E10)
IC <- c(1,0,0)
params <- c(0.04, 10000, 30000000)
reltol <- 1e-04
abstol <- c(1e-8,1e-14,1e-6)

## Solving the ODEs using cvode function
df1 <- cvode(time_vec, IC, ODE_R , params, reltol, abstol)           ## using R
df2 <- cvode(time_vec, IC, ODE_Rcpp , params, reltol, abstol)        ## using Rcpp

## Check that both solutions are identical
# identical(df1, df2)
```

cvodes *cvodes*

Description

CVODES solver to solve ODEs and calculate sensitivities

Usage

```
cvodes(
  time_vector,
  IC,
  input_function,
  Parameters,
  reltolerance = 1e-04,
  abstolerance = 1e-04,
  SensType = "STG",
  ErrCon = "F"
)
```

Arguments

`time_vector`	time vector
`IC`	Initial Conditions
`input_function`	Right Hand Side function of ODEs
`Parameters`	Parameters input to ODEs
`reltolerance`	Relative Tolerance (a scalar, default value = 1e-04)
`abstolerance`	Absolute Tolerance (a scalar or vector with length equal to ydot, default = 1e-04)
`SensType`	Sensitivity Type - allowed values are Staggered (default)", "STG" (for Staggered) or "SIM" (for Simultaneous)
`ErrCon`	Error Control - allowed values are TRUE or FALSE (default)

Examples

```
# Example of solving a set sensitivity equations for ODEs with cvodes function
# ODEs described by an R function
ODE_R <- function(t, y, p){

  # vector containing the right hand side gradients
  ydot = vector(mode = "numeric", length = length(y))

  # R indices start from 1
  ydot[1] = -p[1]*y[1] + p[2]*y[2]*y[3]
  ydot[2] = p[1]*y[1] - p[2]*y[2]*y[3] - p[3]*y[2]*y[2]
  ydot[3] = p[3]*y[2]*y[2]

  # ydot[1] = -0.04 * y[1] + 10000 * y[2] * y[3]
  # ydot[3] = 30000000 * y[2] * y[2]
  # ydot[2] = -ydot[1] - ydot[3]

  ydot
}

# ODEs can also be described using Rcpp
Rcpp::sourceCpp(code = '

                #include <Rcpp.h>
                using namespace Rcpp;

                // ODE functions defined using Rcpp
                // [[Rcpp::export]]
                NumericVector ODE_Rcpp (double t, NumericVector y, NumericVector p){

                // Initialize ydot filled with zeros
                NumericVector ydot(y.length());

                ydot[0] = -p[0]*y[0] + p[1]*y[1]*y[2];
                ydot[1] = p[0]*y[0] - p[1]*y[1]*y[2] - p[2]*y[1]*y[1];
                ydot[2] = p[2]*y[1]*y[1];

                return ydot;

                }')



# R code to genrate time vector, IC and solve the equations
time_vec <- c(0.0, 0.4, 4.0, 40.0, 4E2, 4E3, 4E4, 4E5, 4E6, 4E7, 4E8, 4E9, 4E10)
IC <- c(1,0,0)
params <- c(0.04, 10000, 30000000)
reltol <- 1e-04
abstol <- c(1e-8,1e-14,1e-6)

## Solving the ODEs and Sensitivities using cvodes function
df1 <- cvodes(time_vec, IC, ODE_R , params, reltol, abstol,"STG",FALSE)         ## using R
df2 <- cvodes(time_vec, IC, ODE_Rcpp , params, reltol, abstol,"STG",FALSE)      ## using Rcpp

## Check that both solutions are identical
# identical(df1, df2)
```

cvsolve *cvsolve*

Description

CVSOLVE solver to solve stiff ODEs with discontinuties

Usage

```
cvsolve(
  time_vector,
  IC,
  input_function,
  Parameters,
  Events = NULL,
  reltolerance = 1e-04,
  abstolerance = 1e-04
)
```

Arguments

`time_vector`	time vector
`IC`	Initial Conditions
`input_function`	Right Hand Side function of ODEs
`Parameters`	Parameters input to ODEs
`Events`	Discontinuities in the solution (a DataFrame, default value is NULL)
`reltolerance`	Relative Tolerance (a scalar, default value = 1e-04)
`abstolerance`	Absolute Tolerance (a scalar or vector with length equal to ydot, default = 1e-04)

Examples

```
# Example of solving a set of ODEs with multiple discontinuities using cvsolve
# A simple One dimensional equation, y = -0.1 * y
# ODEs described by an R function
ODE_R <- function(t, y, p){

  # vector containing the right hand side gradients
  ydot = vector(mode = "numeric", length = length(y))

  # R indices start from 1
  ydot[1] = -p[1]*y[1]

  ydot

}

# R code to generate time vector, IC and solve the equations
TSAMP <- seq(from = 0, to = 100, by = 0.1)      # sampling time points
IC <- c(1)
params <- c(0.1)

# A dataset describing the dosing at times at which additions to y[1] are to be done
# Names of the columns don't matter, but they MUST be in the order of state index,
# times and Values at discontinuity.
TDOSE <- data.frame(ID = 1, TIMES = c(0, 10, 20, 30, 40, 50), VAL = 100)
df1 <- cvsolve(TSAMP, c(1), ODE_R, params)         # solving without any discontinuity
df2 <- cvsolve(TSAMP, c(1), ODE_R, params, TDOSE)  # solving with discontinuity
```

ida *ida*

Description

IDA solver to solve stiff DAEs

Usage

```
ida(
  time_vector,
  IC,
  IRes,
  input_function,
  Parameters,
  reltolerance = 1e-04,
  abstolerance = 1e-04
)
```

Arguments

`time_vector`	time vector
`IC`	Initial Value of y
`IRes`	Inital Value of ydot
`input_function`	Right Hand Side function of DAEs
`Parameters`	Parameters input to ODEs
`reltolerance`	Relative Tolerance (a scalar, default value = 1e-04)
`abstolerance`	Absolute Tolerance (a scalar or vector with length equal to ydot, default = 1e-04)

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